

A classification of spin 1/2 matrix product states with two dimensional auxiliary matrices

Marzieh Asoudeh ¹ †

Department of Physics, Shahid Beheshti University, GC
19839-63113, Tehran, Iran

Abstract

We classify the matrix product states having only spin-flip and parity symmetries, which can be constructed from two dimensional auxiliary matrices. We show that there are three distinct classes of such states and in each case, we determine the parent Hamiltonian and the points of possible quantum phase transitions. For two of the models, the interactions are three-body and for one the interaction is two-body.

PACS Number:75.10.Jm

¹*m – asoudeh@sbu.ac.ir*

1 Introduction

The problem of determining the ground state of a given many-body Hamiltonian, is an important problem in condensed matter and mathematical physics. There is already a rich literature on this subject, which dates back to the work of Hans Bethe on the Heisenberg spin chain and has continued since then with the works of many other people including Yang, Baxter, and Lieb, to name only a few. In particular for spin systems, the exponential increase in the dimension of Hilbert space of such a system, as the number of particles rise, turns this problem into a computationally formidable one, beyond the capability of any classical computer. In fact it has now been established that finding the ground state of a given many-body Hamiltonian is the analog of NP-complete problems for quantum computers [1]. The lesson that we learn from all this is that it is highly improbable that we be able to find a generic system with exactly known ground state. Nevertheless, there are systems with exactly known ground states and even if such systems are not exactly what we have in nature or in the laboratories, they may be good approximations to real systems, or at least may teach us useful and important concepts and methods for studying more realistic systems.

One of the methods, developed in recent years, for investigating this problem is the Matrix Product State or Finitely Correlated State [2, 3, 4] formalism. It is also called Optimal Ground State formalism in some references [5, 6, 7]. The main theme is that one starts with a state with prescribed symmetries and properties, and then construct the family of Hamiltonians for which this state is an exact ground state. It is obvious that for any given state $|\psi\rangle$, the equation $H|\psi\rangle = 0$ has always many solutions for the unknown H , since the number of equations is much less than the number of unknowns. However the problem becomes interesting and quite non-trivial when we put physical constraints on the Hamiltonian. That is we demand that i) H be positive, so that $|\Psi\rangle$ is actually the ground state and not an ordinary eigenstate, ii) that it be a sum of local terms, i.e. $H = \sum_k h_{k,k+l}$, where $h_{k,k+l}$ acts on a block of $l+1$ spins, and iii) that both the state and the Hamiltonian have some reasonable physical symmetries, like parity, spin-flip, and at times rotational symmetries.

In the past few years, a lot of interest has been attracted to the subject of matrix product states [8, 9, 10, 11, 12, 13], specially after the emergence of the field of quantum information [14, 15, 16, 17, 18]. The reason is the complementary role that the fields of condensed matter physics and quantum information play in investigation of many body systems. On the one hand quantum information starts with properties of states, while condensed matter physics, starts from the properties of the Hamiltonian which embodies the interactions and energy of the system. The matrix product formalism is one of the subjects which lies at the borderline of these two subjects.

As is well known, in this formalism, one starts from proposed states whose expansion coefficients are the trace of product of given matrices. While for numerical investigations, i.e. the density matrix renormalization group (DMRG), one usually

starts from large dimensional matrices, to simulate ground states of given Hamiltonians, in the approach which is used for finding exactly solvable models, one starts from low dimensional matrices and finds Hamiltonians for which these states are exact ground states. This is the approach which has been used in our works and in many other works in the past few years [8, 9, 10, 11, 12, 13, 19, 20, 21, 22, 23, 24, 25]. In this article we follow this approach and classify all the matrix product states which can be constructed from two dimensional matrices. We restrict ourselves to states which allow one or another of the spin-flip or parity symmetries and find that there are three classes of such matrix product states. We will study these states and find the parent Hamiltonians and also the points or lines in the space of control parameters where a MPS-quantum phase transition [26] (MPS-QPT) may occur. This is a term, introduced in [27] to differentiate these kinds of QPT's (characterized by any discontinuity in any macroscopic quantity) from the conventional QPT,s in which a non-analyticity in the ground state energy typically occurs.

The structure of this paper is as follows: To make the article self-contained, in the next section we briefly introduce the basic elements of the formalism. In section (3) we discuss the symmetry properties of MPS and classify the spin 1/2 states with two dimensional matrices. We show that there are three classes, denoted by a model A, model B and model C and studied in subsequent sections. We end the paper with a discussion.

2 A brief introduction to matrix product states

First let us review the basics of matrix product states. Consider a homogeneous ring of N sites, where each site describes a d -level state. The Hilbert space of each site is spanned by the basis vectors $|i\rangle$, $i = 0, \dots, d-1$. A state

$$|\Psi\rangle = \sum_{i_1, i_2, \dots, i_N} \psi_{i_1 i_2 \dots i_N} |i_1, i_2, \dots, i_N\rangle \quad (1)$$

is called a matrix product state if there exists D dimensional complex matrices $A_i \in C^{D \times D}$, $i = 0 \dots d-1$ such that

$$\psi_{i_1, i_2, \dots, i_N} = \frac{1}{\sqrt{Z}} \text{tr}(A_{i_1} A_{i_2} \cdots A_{i_N}), \quad (2)$$

where Z is a normalization constant given by

$$Z = \text{tr}(E^N) \quad (3)$$

and

$$E := \sum_{i=0}^{d-1} A_i^* \otimes A_i. \quad (4)$$

Here we are restricting ourselves to translationally invariant states, by taking the matrices to be site-independent. By defining the vector valued matrix

$$\mathcal{A} = \sum_{i=1}^d A_i |i\rangle, \quad (5)$$

one can write the MPS in a more concise way as

$$|\psi\rangle = \text{tr}(\mathcal{A} \otimes \mathcal{A} \otimes \cdots \otimes \mathcal{A}), \quad (6)$$

where we use the convention

$$\text{tr}(\mathcal{A} \otimes \mathcal{A}) := \text{tr}(A_i A_j) |i\rangle \otimes |j\rangle.$$

It is important to note that the MPS representation (2) is not unique and a transformation such as

$$A_i \longrightarrow \mu U A_i U^{-1} \quad (7)$$

where U is an invertible matrix, and μ is a constant, leaves the state invariant. The simple structure of the MPS allows also an easy calculation of correlation functions. Let O be any local operator acting on a single site. Then we can obtain the one-point function on site k of the chain $\langle \Psi | O(k) | \Psi \rangle$ as follows:

$$\langle \Psi | O(k) | \Psi \rangle = \frac{\text{tr}(E^{k-1} E_O E^{N-k})}{\text{tr}(E^N)}, \quad (8)$$

where

$$E_O := \sum_{i,j=0}^{d-1} \langle i | O | j \rangle A_i^* \otimes A_j. \quad (9)$$

In the thermodynamic limit $N \rightarrow \infty$, equation (8) gives

$$\langle \Psi | O | \Psi \rangle = \frac{\langle \lambda_{\max} | E_O | \lambda_{\max} \rangle}{\lambda_{\max}}, \quad (10)$$

where we have used the translation invariance of the model and λ_{\max} is the eigenvalue of E with the largest absolute value and $|\lambda_{\max}\rangle$ and $\langle \lambda_{\max}|$ are the right and left eigenvectors corresponding to this eigenvalue, normalized such that $\langle \lambda_{\max} | \lambda_{\max} \rangle = 1$. Here we are assuming that the largest eigenvalue of E is non-degenerate. In case λ_{\max} is degenerate with degree equal to g , then Eq. (10) will be modified to

$$\langle \Psi | O | \Psi \rangle = \frac{\sum_{i=1}^g \langle \lambda_{\max,i} | E_O | \lambda_{\max,i} \rangle}{\lambda_{\max}}, \quad (11)$$

The n-point functions can be obtained in a similar way. For example, the two-point function $\langle \Psi | O(k) O(l) | \Psi \rangle$ can be obtained as

$$\langle \Psi | O(k) O(l) | \Psi \rangle = \frac{\text{tr}(E_O(k) E_O(l) E^N)}{\text{tr}(E^N)} \quad (12)$$

where $E_O(k) := E^{k-1} E_O E^{-k}$. Note that this is a formal notation which allows us to write the n-point functions in a uniform way, it does not require that E be an invertible matrix. In the thermodynamic limit the two point function turns out to be

$$\langle \Psi | O(1) O(r) | \Psi \rangle = \frac{1}{\lambda_{\max}^r} \sum_i \lambda_i^{r-2} \langle \lambda_{\max} | E_O | \lambda_i \rangle \langle \lambda_i | E_O | \lambda_{\max} \rangle. \quad (13)$$

For large distances $r \gg 1$, this formula reduces to

$$\langle \Psi | O(1)O(r) | \Psi \rangle - \langle \Psi | O | \Psi \rangle^2 = \frac{\lambda_1^{r-2}}{\lambda_{max}^r} \langle \lambda_{max} | E_O | \lambda_1 \rangle \langle \lambda_1 | E_O | \lambda_{max} \rangle, \quad (14)$$

where λ_1 is the second largest eigenvalue of E for which the matrix element $\langle \lambda_1 | E_O | \lambda_{max} \rangle$ is non-vanishing and we have assumed that the eigenvectors of E have been normalized, i.e. $\langle \lambda_i | \lambda_j \rangle = \delta_{ij}$. Thus the correlation length is given by

$$\xi = \frac{1}{\ln \frac{\lambda_{max}}{\lambda_1}}. \quad (15)$$

Any level crossing in the largest eigenvalue of the matrix E signals a possible MPS-QPT. Here we are using the term quantum phase transition in a broader sense than usual [27], that is, we call any discontinuity in any macroscopic quantity a quantum phase transition, even if the ground state energy itself is a continuous function of the coupling constants. Also, due to (15), any level crossing in the second largest eigenvalue of E implies the correlation length of the system has undergone a discontinuous change.

2.1 The Hamiltonian

Given a matrix product state, the reduced density matrix of k consecutive sites is given by

$$\rho_{i_1 \dots i_k, j_1 \dots j_k} = \frac{\text{tr}((A_{i_1}^* \dots A_{i_k}^* \otimes A_{j_1} \dots A_{j_k}) E^{N-k})}{\text{tr}(E^N)}. \quad (16)$$

The null space of this reduced density matrix includes the solutions of the following system of equations

$$\sum_{j_1, \dots, j_k=0}^{d-1} c_{j_1 \dots j_k} A_{j_1} \dots A_{j_k} = 0. \quad (17)$$

Given that the matrices A_i are of size $D \times D$, there are D^2 equations with d^k unknowns. Since there can be at most D^2 independent equations, there are at least $d^k - D^2$ solutions for this system of equations. Thus for the density matrix of k sites to have a null space it is sufficient that the following inequality holds

$$d^k > D^2. \quad (18)$$

Let the null space of the reduced density matrix be spanned by the orthogonal vectors $|e_\alpha\rangle$, ($\alpha = 1, \dots, s, \geq d^k - D^2$). Then we can construct the local hamiltonian acting on k consecutive sites as

$$h := \sum_{\alpha=1}^s \mu_\alpha |e_\alpha\rangle \langle e_\alpha|, \quad (19)$$

where μ_α 's are positive constants. These parameters together with the parameters of the vectors $|e_i\rangle$ inherited from those of the original matrices A_i , determine the total number of coupling constants of the Hamiltonian. If we call the embedding of this

local Hamiltonian into the sites l to $l+k$ by $h_{l,l+k}$ then the full Hamiltonian on the chain is written as

$$H = \sum_{l=1}^N h_{l,l+k}. \quad (20)$$

The state $|\Psi\rangle$ is then a ground state of this hamiltonian with vanishing energy. The reason is as follows:

$$\langle \Psi | H | \Psi \rangle = \text{tr}(H|\Psi\rangle\langle\Psi|) = \sum_{l=1}^N \text{tr}(h_{l,l+k}\rho_{l,l+k}) = 0, \quad (21)$$

where $\rho_{l,k+l}$ is the reduced density matrix of sites l to $l+k$ and in the last line we have used the fact that h is constructed from the null eigenvectors of ρ for k consecutive sites. Given that H is a positive operator, this proves the assertion.

In view of the above introduction, we have a clear recipe for constructing matrix product states and a family of parent Hamiltonians. First one chooses the matrices throwing away all spurious degrees of freedom by transformations (7) and reducing further the degrees of freedom by imposing symmetries. In this way one ends with a reasonable set of matrix product states, which hopefully may have applications in description of real physical systems. Imposing a continuous symmetry, like rotation around an axis, restricts the matrices considerably [8, 9, 10]. In this article we restrict ourselves to discrete symmetries only which allow a larger variety of models to be constructed. For two dimensional auxiliary matrices, this is a simple tractable problem, which we do in this article. For larger matrices, the problem is not so simple and we defer it to another work.

3 The classification of 2 dimensional matrices for matrix product states of spin 1/2 chains

We now classify all the two dimensional matrices which can be used for constructing spin 1/2 matrix product states. We restrict ourselves to the case where these states have spin-flip and left-right symmetries.

3.1 Symmetries

Consider now a local symmetry operator R acting on a site as $R|i\rangle = R_{ji}|j\rangle$ where summation convention is being used. R is a d dimensional unitary representation of the symmetry. A global symmetry operator $\mathcal{R} := R^{\otimes N}$ will then change this state to another matrix product state

$$\Psi_{i_1 i_2 \dots i_N} \longrightarrow \Psi' := \text{tr}(A'_{i_1} A'_{i_2} \cdots A'_{i_N}), \quad (22)$$

where

$$A'_i := R_{ij}A_j. \quad (23)$$

A sufficient but not necessary condition for the state $|\Psi\rangle$ to be invariant under this symmetry is that there exist an operator $U(R)$ such that

$$R_{ij}A_j = U(R)A_iU^{-1}(R). \quad (24)$$

Thus R and $U(R)$ are two unitary representations of the symmetry, respectively of dimensions d and D . Equation (24) will be our guiding lines in defining states with prescribed symmetries. Spin-flip symmetry means that

$$\psi_{\overline{i_1}, \overline{i_2}, \dots, \overline{i_N}} = \psi_{i_N, i_{N-1}, \dots, i_1}, \quad (25)$$

where $\overline{i} = 1 - i$. For a matrix product state, this requires that there be a matrix like X , such that

$$XA_0X^{-1} = \epsilon A_1, \quad XA_1X^{-1} = \epsilon A_0, \quad (26)$$

where $\epsilon = \pm 1$. Similarly left-right symmetry means that

$$\psi_{i_1, i_2, \dots, i_N} = \psi_{i_N, i_{N-1}, \dots, i_1}. \quad (27)$$

For a matrix product state, this means that there be a matrix Ω such that

$$\Omega A_0 \Omega^{-1} = \sigma A_0^T, \quad \Omega A_1 \Omega^{-1} = \sigma A_1^T, \quad (28)$$

where the superscript T stands for the transpose and $\sigma = \pm 1$. These conditions are general irrespective of the dimension of matrices. For two dimensional matrices however, if we take the trace and determinants of both sides of equations (26) and (28), and comparing them, we find that

$$\text{tr}(A_0) = \epsilon \text{tr}(A_1), \quad (29)$$

and

$$\det(A_0) = \det(A_1). \quad (30)$$

The important point is that for two dimensional matrices, the trace and determinant are the only invariants under similarity transformations, and hence these two equations allow us to classify all the matrices A_0 and A_1 which can be used for construction of spin 1/2 matrix product states. We will use the freedom (7) and also the above two conditions to show that there are three distinct classes of matrix pairs and corresponding matrix product states. In the next three sections, we introduce the matrix pairs and study the properties of the matrices obtained from them. For ease of distinction, we use different notations for the matrix pairs in each section, namely we denote the matrix pairs by A_i , B_i and C_i in the following sections.

4 Model A

If one of the matrices say A_0 is diagonalizable, we can use freedom in re-scaling $A_0 \rightarrow \mu A_0$ to put it in the form

$$A_0 = \begin{pmatrix} 1+g & 0 \\ 0 & 1-g \end{pmatrix}, \quad (31)$$

where g is a free parameter. Now take A_1 as an arbitrary matrix of the form $A_1 = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$. If $bc \neq 0$, then we can use the transformation (7) with $U = \begin{pmatrix} \sqrt{c} & \sqrt{b} \\ \sqrt{b} & \sqrt{d} \end{pmatrix}$ and a further re-definition of $\sqrt{bc} \rightarrow b$ to put it in the form

$$A_1 = \begin{pmatrix} a & b \\ b & d \end{pmatrix}. \quad (32)$$

For this type of matrices, the MPS is automatically left-right symmetric, with $\Omega = I$. From equations (29) and (30), we find the following constraints on the parameters,

$$1 - g^2 = (ad - b^2) \quad 2\epsilon = (a + d). \quad (33)$$

To solve the second equation, we put

$$a = \epsilon + u, \quad b = \epsilon - u, \quad (34)$$

which turns the first equation into

$$g^2 = b^2 + u^2, \quad (35)$$

which can be solved by the parametrization $u = g \cos \theta$ and $b = g \sin \theta$. Therefore the final form of the matrices will be as follows:

$$A_0 = \begin{pmatrix} 1+g & 0 \\ 0 & 1-g \end{pmatrix}, \quad A_1 = \begin{pmatrix} \epsilon + g \cos \theta & g \sin \theta \\ g \sin \theta & \epsilon - g \cos \theta \end{pmatrix}. \quad (36)$$

The matrices satisfy the symmetry constraints (26) and (28) with $\Omega = I$ and

$$X = \begin{pmatrix} \epsilon \sin \theta & -\epsilon \sin \theta \\ 1 - \epsilon \cos \theta & 1 + \epsilon \cos \theta \end{pmatrix}. \quad (37)$$

We now restrict ourselves to the case $\epsilon = 1$ (We do this also for other models B and C). To study the properties of the corresponding MPS, we should determine the eigenvalues of the transition matrix $E_A := A_0 \otimes A_0 + A_1 \otimes A_1$. For general values of the parameters, the analytical form of these eigenvalues are complicated. However we can gain insight by looking at them for generic values of the parameter g . Figure (4) shows the eigenvalues as a function of θ for two values of the parameter g . The same pattern repeats for other values of g . We first see that there is no level-crossing in the largest eigenvalue and hence no MPS quantum phase transition in this model. However for every value of g , two points are important. The point $\theta = \Pi$ (or $-\Pi$), is the point where the largest and the next to largest eigenvalues become equal. This is a point where according to (15), the correlation length becomes infinite. It is seen from (36) that at this point, the matrices become diagonal $A_0 = \text{diagonal}(1+g, 1-g)$ and $A_1 = \text{diagonal}(1-g, 1+g)$ and according to (6), the un-normalized state becomes the sum of two product states, namely

$$|\psi\rangle = |\phi_+\rangle^{\otimes N} + |\phi_-\rangle^{\otimes N}, \quad (38)$$



Figure 1: (Color Online) The eigenvalues of the transition matrix E_A for $\epsilon = 1$ and a generic value of g (i.e. $g=1/2$) as a function of θ .

where

$$|\phi_+\rangle = (1+g)|0\rangle + (1-g)|1\rangle, \quad |\phi_-\rangle = (1-g)|0\rangle + (1+g)|1\rangle. \quad (39)$$

Let us now find the parent Hamiltonian for a fixed value of the parameter g , say $g = 1$. To this end, we have to see for which value of k (the range of interaction), the system of equations (17) have a non-trivial solution. It is seen that the smallest k for which there is such a solution is $k = 3$.

The solution space of this system of equations turn out to be spanned by the following vectors:

$$|e_1^A\rangle = -\frac{1+\cos(\theta)}{2}|000\rangle + |101\rangle, \quad (40)$$

$$|e_2^A\rangle = |001\rangle - |011\rangle \quad (41)$$

$$|e_3^A\rangle = |100\rangle - |110\rangle \quad (42)$$

$$|e_4^A\rangle = |010\rangle - \frac{1+\cos(\theta)}{2}|111\rangle. \quad (43)$$

The symmetries of the parent Hamiltonian now show itself in the form that the above states, which transform into each other under the action of these symmetries. To have a Hamiltonian which respects these symmetries, we construct it as follows:

$$h_A = J(|e_1^A\rangle\langle e_1^A| + |e_4^A\rangle\langle e_4^A|) + K(|e_2^A\rangle\langle e_2^A| + |e_3^A\rangle\langle e_3^A|). \quad (44)$$

The final form of the the full Hamiltonian in terms of Pauli matrices, after neglecting additive and multiplicative constants becomes

$$\begin{aligned} H_A &= \sum_{i=1}^N J_1 \sigma_i^z \sigma_{i+1}^z + J_2 \sigma_i^z \sigma_{i+2}^z - u J \sigma_i^x \sigma_{i+2}^x + u J \sigma_i^y \sigma_{i+2}^y \\ &- \frac{K}{2} \sigma_i^x + \frac{K}{2} \sigma_i^z \sigma_{i+1}^x \sigma_{i+2}^z, \end{aligned} \quad (45)$$

where $u = \frac{1+\cos\theta}{2}$ and

$$J_1 = J \frac{u^2 - 1}{2}, \quad (46)$$

$$J_2 = J \frac{u^2 + 1}{2} - \frac{K}{2}. \quad (47)$$

This is a three-body Hamiltonian with two free coupling constants. We will say more about this in the discussion.

5 Model B

In accordance with our proposed notation, we denote the matrices in this case by B_0 and B_1 . In this case the matrices are the same as in the previous case, except that one of the parameters, say b is zero. There is no transformation which can put B_1 into symmetric form, and we have

$$B_1 = \begin{pmatrix} a & 0 \\ c & d \end{pmatrix}. \quad (48)$$

In this case no similarity transformation can put the matrix B_1 into symmetric form, without destroying the diagonal form of B_0 and hence the MPS will not be parity invariant or left-right symmetric. From Eqs. (29) and (30), we find that

$$1 - g^2 = ad \quad 2\epsilon = a + d, \quad (49)$$

which lead to the following final parametrization for the matrices, where for definiteness we will show the matrices by a different letter

$$B_0 = \begin{pmatrix} 1+g & 0 \\ 0 & 1-g \end{pmatrix}, \quad B_1 = \begin{pmatrix} \epsilon+g & 0 \\ c & \epsilon-g \end{pmatrix}. \quad (50)$$

In this case again we have two free parameters in the MPS state, namely c and g . Moreover the matrices satisfy the spin flip symmetry condition (26) with

$$X = \frac{1+\epsilon}{2} \begin{pmatrix} 2g & 0 \\ c & 1 \end{pmatrix} + \frac{1-\epsilon}{2} \begin{pmatrix} 0 & 2g \\ 1 & c \end{pmatrix}, \quad (51)$$

while they do not have any symmetry under parity (i.e. there is no matrix Ω satisfying (28)).

The eigenvalues of the transition matrix $E_B = B_0 \otimes B_0 + B_1 \otimes B_1$, (for the case $\epsilon = 1$) now become

$$\lambda_1^B = 2(1+g)^2, \quad \lambda_2^B = 2(1-g)^2, \quad \lambda_{3,4}^B = 2(1-g^2), \quad (52)$$

independent of the value of c . Figure (5), shows these eigenvalues as a function of the parameter g . From this figure, a few features can be recognized. First we note that at $g = 0$, there is a crossover between the largest and the second-largest eigenvalues. This points to a possible MPS-quantum phase transition at this point. Furthermore at $g = \pm 1$, there is a discontinuity in the derivative of the second largest eigenvalue which points to a discontinuity in the derivative of the correlation length. In view of the general and rather broad definition of MPS quantum phase transition, as the appearance of any discontinuity of a macroscopic observable, these points are also points of MPS-QPT's. Moreover since the eigenvalues do not depend on the parameter c , it appears that the above points are really lines in the space of coupling constants c and g .

From (36), it is clear that at $g = 0$, the un-normalized MPS turns into the following state

$$|\psi_B\rangle = |\chi_+\rangle^{\otimes N} + |\chi_-\rangle^{\otimes N}, \quad (53)$$

where

$$|\chi_\pm\rangle = (1 \pm g)|0\rangle + |1\rangle. \quad (54)$$

Finally we come to the parent Hamiltonian. For this model we find that the smallest value of k for which the system of equations (17) has a non-trivial solution is $k = 2$ and hence we can have a two-local parent Hamiltonian. The solution space of the system of equations (17) is spanned by the vectors

$$|e_1^B\rangle = -\frac{1}{2}(1+g)|00\rangle + |01\rangle + \frac{1}{2}(g-1)|11\rangle \quad (55)$$

$$|e_2^B\rangle = -\frac{1}{2}(1+g)|11\rangle + |10\rangle + \frac{1}{2}(g-1)|00\rangle. \quad (56)$$

Interestingly we note that the above vectors transform into each other under spin-flip, but they do not have any transformation property under parity which is to be expected, since the original matrices had only spin-flip symmetry. The parent Hamiltonian which is symmetric under spin flip will be

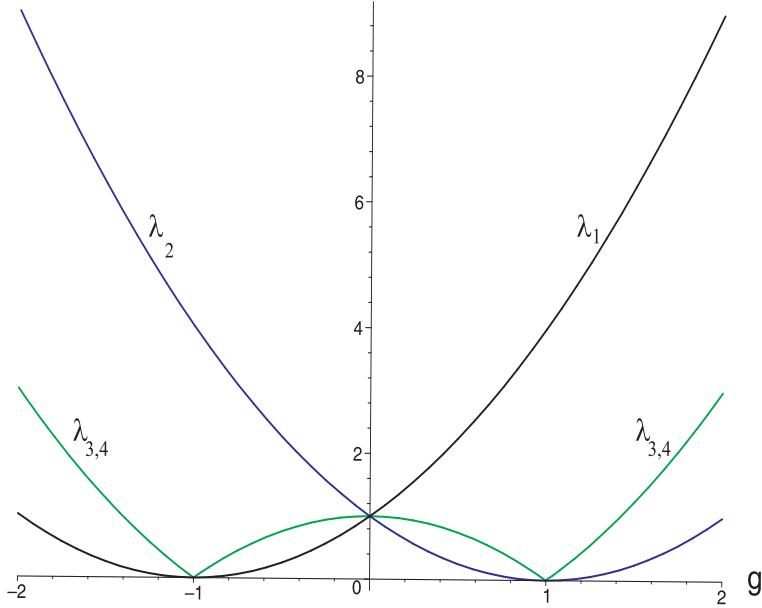


Figure 2: (Color Online) The absolute values of the eigenvalues of the transition matrix E_B for $\epsilon = 1$, as a function of g .

$$h_B = J(|e_1^B\rangle\langle e_1^B| + |e_2^B\rangle\langle e_2^B|) \quad (57)$$

and the full Hamiltonian will be (after neglecting additive and multiplicative constants and collecting all the various terms)

$$H^B = \sum_{i=1}^N (1-g^2)(\sigma_i^x \sigma_{i+1}^x - \sigma_i^y \sigma_{i+1}^y) + \frac{1+2g^2}{2} \sigma_i^z \sigma_{i+1}^z + \sigma_i^x. \quad (58)$$

This is the Heisenberg XYZ system with specific couplings, that is we have found exact solution on a submanifold in the space of couplings. Note that since the Hamiltonian does not depend on the parameter c , while the MPS does, this means that there is a large degeneracy in the ground state. Expansion of the MPS in terms of the parameter c , i.e. $|\Psi(c, g)\rangle = \sum_n c^n |\psi_n(g)\rangle$, will yield the multitude of degenerate ground states $|\psi_n(g)\rangle$ as in [28].

6 Model C

Denoting the matrices by C_0 and C_1 , this is the only remaining case, where C_0 is not diagonalizable and can be put only in the Jordan form

$$C_0 = \begin{pmatrix} 1 & 0 \\ g & 1 \end{pmatrix}. \quad (59)$$

We take the general form of C_1 to be $C_1 = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ and impose the conditions (29) and (30), from which we obtain the constraints

$$a + d = 2\epsilon \quad (60)$$

$$ad - bc = 1. \quad (61)$$

The first constraint is solved by the parametrization $a = \epsilon + u$ and $d = \epsilon - u$, which when inserted into the second equation, gives $u^2 + bc = 0$, the solution of which is $b = \mu u$ and $c = -\frac{u}{\mu}$. However the parameter μ can be set to unity by a gauge transformation $C_i \rightarrow UC_iU^{-1}$ with $U = \begin{pmatrix} 1 & 0 \\ 0 & \mu \end{pmatrix}$. Thus the final form of the matrices become

$$C_0 = \begin{pmatrix} 1 & 0 \\ g & 1 \end{pmatrix}, \quad C_1 = \begin{pmatrix} \epsilon + u & u \\ -u & \epsilon - u \end{pmatrix}. \quad (62)$$

One can verify the existence of both symmetries, with matrices

$$X = \begin{pmatrix} u & u \\ g & 0 \end{pmatrix} \quad \text{and} \quad \Omega = \begin{pmatrix} 0 & 1 \\ 1 & -2 \end{pmatrix}, \quad (63)$$

such that

$$X^{-1}C_iX = C_{\bar{i}}, \quad \Omega^{-1}C_i\Omega = C_i^T. \quad (64)$$

The eigenvalues of the transfer matrix $E_C = C_0 \otimes C_0 + C_1 \otimes C_1$, are found to be

$$\lambda_1^C = 2, \quad \lambda_2^C = 2 - ug, \quad \lambda_{\pm}^C = 2 + \frac{ug}{2} \pm \frac{1}{2}\sqrt{16ug + u^2g^2}. \quad (65)$$

Figure (6) shows the largest eigenvalue of the transfer matrix in the $u - g$ plane. It is seen that the lines $u = 0$ and $g = 0$ are the crossover lines where the largest eigenvalue changes and hence an MPS-QPT (MPS quantum phase transition) is expected to occur on these lines.

Finally we can find the parent Hamiltonian of this model. The system of equations (17) has a nontrivial solution for $k = 3$ and the solution space is spanned by the vectors:

$$\begin{aligned} |e_1^C\rangle &= |001\rangle + |110\rangle - |011\rangle - |100\rangle \\ |e_2^C\rangle &= (1 + ug)(|000\rangle + |111\rangle) + (|001\rangle + |011\rangle + |100\rangle + |110\rangle) - 3(|010\rangle + |101\rangle) \\ |e_3^C\rangle &= 2(|000\rangle - |111\rangle) - 3(|001\rangle - |011\rangle + |100\rangle - |110\rangle) \end{aligned}$$

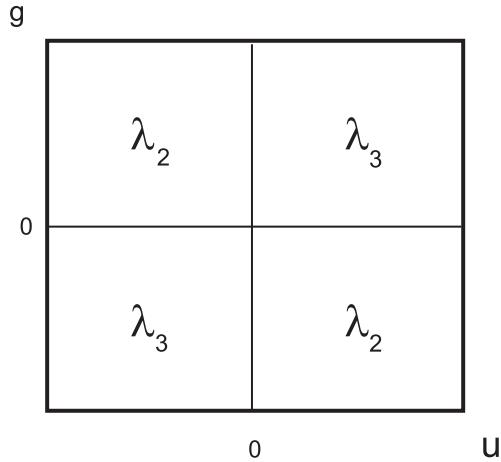


Figure 3: (Color Online) The largest eigenvalue of transfer matrix for model III. There are two crossover lines for the largest magnitude eigenvalue.

$$|e_4^C\rangle = 2(|010\rangle - |101\rangle) - (1 + ug)(|001\rangle - |011\rangle + |100\rangle - |110\rangle) \quad (66)$$

The interesting point about these vectors is that all of them are invariant (modulo a sign) under the parity and spin-flip transformations and hence the symmetric Hamiltonian can be written in the following form, with four free coupling constants:

$$h_C = \sum_{i=1}^4 J_i |e_i^C\rangle \langle e_i^C|. \quad (67)$$

The explicit expression of the total Hamiltonian can be obtained along the same lines as for model A and model B. We will not do it here.

7 Discussion

In the formalism of matrix product states, there is a large room for constructing states and parent Hamiltonians. What really constrains this freedom and guides us along a way which may lead to interesting states and Hamiltonians is consideration of symmetries. The other constraining elements is the dimension of matrices which we choose. In this article we have classified all such states which are constructed from two dimensional matrices and have two important symmetries, namely the spin flip symmetry and the parity symmetry. We have shown that there are three different models, two of which lead to parent Hamiltonians with nearest and next-nearest interaction (models A and C) while one of them lead to a Hamiltonian with nearest neighbor interaction (model B). Furthermore, by calculating the eigenvalues of the transfer matrix in each case and determining the points of crossover between the largest and the next to largest eigenvalues of this matrix, we have identified the points of possible MPS quantum phase transitions. While in many of the works which have been reported on model building in matrix product states, [8, 9, 10, 19, 20, 21, 22, 23],

rotation symmetry has been taken into account, a condition which highly restricts the form of matrices, in this article we have relaxed this continuous symmetry in order to find all models compatible with discrete symmetries in order exhaust all the possibilities with two dimensional matrices. Any model with these symmetries must be equivalent to one of the above three models. For example in [27], the following model was suggested

$$A'_0 = \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}, \quad A'_1 = \begin{pmatrix} 1 & q \\ 0 & 0 \end{pmatrix}, \quad (68)$$

which has spin-flip symmetry with $X = \begin{pmatrix} 0 & q \\ 1 & 0 \end{pmatrix}$. The Hamiltonian for this model is [27]

$$H = \sum_{i=1}^N 2(q^2 - 1)\sigma_i^z\sigma_{i+1}^z - (1+q)^2\sigma_i^x + (q-1)^2\sigma_i^z\sigma_{i+1}^x\sigma_{i+2}^z. \quad (69)$$

It is easy to see that this model is equivalent to model A above. In fact the transformation

$$SA_i(g=1)S^{-1} = 2A'_i$$

with $S = \begin{pmatrix} 0 & \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} & -\cos \frac{\theta}{2} \end{pmatrix}$ in which $q = \frac{1+\cos \theta}{2}$, proves the equivalence.

8 Acknowledgements

I would like to thank V. Karimipour for valuable discussion and comments.

References

- [1] M. A. Nielsen, and I. L. Chuang; *Quantum computation and quantum information*, Cambridge University Press, Cambridge, 2000.
- [2] M. Fannes, B. Nachtergaelle and R. F. Werner, Commun. Math. Phys. **144**, 443 (1992).
- [3] I. Affleck, T. Kennedy, E. H. Lieb, H. Tasaki, Commun.Math. Phys. **115**, 477 (1988);
- [4] A. Klumper, A. Schadschneider and J. Zittartz, J. Phys. A (1991) L293; Z. Phys. B, **87** (1992) 281; Europhys. Lett., **24** (1993) 293.
- [5] H. Niggemann, and J. Zittartz, J. Phys. A: Math. Gen. 31, 9819-9828 (1998).
- [6] E. Bartel, A. Schadschneider and J. Zittartz, Eur. Phys. Jour. B, **31**, 2, 209-216 (2003).

- [7] M. A. Ahrens, A. Schadschneider, and J. Zittartz, *Europhys. Lett.* **59** 6, 889 (2002).
- [8] A. K. Kolezhuk and H. J. Mikeska, *Phys. Rev. Lett.* **80**, 2709 (1998); *Int. J. Mod. Phys. B*, **12**, 2325-2348 (1998).
- [9] A. K. Kolezhuk, H. J. Mikeska, and Shoji Yamamoto, *Phys. Rev. B* **55**, R3336 - R3339 (1997).
- [10] H. Niggemann, A. Klümper, and J. Zittartz, *Eur. Phys. J. B* **13**, 15 (2000).
- [11] J. M. Roman, G. Sierra, J. Dukelsky, and M. A. Martn-Delgado, *J. Phys. A: Mathematical and General*, **31**, 48, 9729-9759(1998).
- [12] H. Niggemann, A. Klümper, and J. Zittartz, *Z. Phys. B* **104**, 103 (1997).
- [13] A. Klümper, S. Matveenko, and J. Zittartz, *Z. Phys. B* **96**, 401 (1995).
- [14] F. Verstraete, D. Porras, J. I. Cirac, *Phys. Rev. Lett.* **93**, 227205 (2004).
- [15] F. Verstraete, J. J. Garcia-Ripoll, and J. I. Cirac, *Phys. Rev. Lett.* **93**, 207204 (2004).
- [16] F. Verstraete, J. I. Cirac, *Phys. Rev. B* **73**, 094423 (2006); T. J. Osborne, *Phys. Rev. Lett.* **97**, 157202 (2006); M. B. Hastings, *Phys. Rev. B* **73**, 085115 (2006).
- [17] G. Vidal, *Phys. Rev. Lett.* **91**, 147902 (2003).
- [18] F. Verstraete, M. A. Martin-Delgado, and J. I. Cirac, *Phys. Rev. Lett.* **92**, 087201 (2004); F. Verstraete, M. Popp, and J. I. Cirac, *Phys. Rev. Lett.* **92**, 027901 (2004); F. Verstraete, J. I. Cirac, J. I. Latorre, E. Rico, and M. M. Wolf, *Phys. Rev. Lett.* **94** 140601(2005).
- [19] M. Asoudeh, V. Karimipour, and A. Sadrolashrafi, *Phys. Rev. A* **76**, 012320 (2007).
- [20] M. Asoudeh, V. Karimipour and A. Sadrolashrafi, *Phys. Rev. B*, **75**, 224427 (2007).
- [21] M. Asoudeh, V. Karimipour, and A. Sadrolashrafi, *Phys. Rev. A* **76**, 012320 (2007).
- [22] S. Alipour, V. Karimipour and L. Memarzadeh, *Phys. Rev. A* **75**, 052322 (2007).
- [23] A. Trebedi and I. Bose, *Phys. Rev. A* **75**, 042304(2007).
- [24] S. Alipour, S. Baghbanzadeh, and V. Karimipour, C *Europhysics Letters (EPL)*, 84 (2008) 67006.
- [25] V. Karimipour and L. Memarzadeh, *Phys. Rev. B* **77**, 094416 (2008).

- [26] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, 1999).
- [27] M. M. Wolf, G. Ortiz, F. Verstraete and I. Cirac, Phys. Rev. Lett. 97, 110403 (2006).
- [28] S. Alipour, V. Karimipour, and L. Memarzadeh, Eur. Phys. J. B 62, 159-169 (2008).